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On ordering bicyclic graphs with respect to the Laplacian spectral radius ☆

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ABSTRACT

A connected graph of order n is bicyclic if it has $n+1$ edges. He et al. [C.X. He, J.Y. Shao, J.L. He, On the Laplacian spectral radii of bicyclic graphs, Discrete Math. 308 (2008) 5981–5995] determined, among the n-vertex bicyclic graphs, the first four largest Laplacian spectral radii together with the corresponding graphs (six in total). It turns that all these graphs have the spectral radius greater than $n-1$. In this paper, we first identify the remaining n-vertex bicyclic graphs (five in total) whose Laplacian spectral radius is greater than or equal to $n-1$. The complete ordering of all eleven graphs in question was obtained by determining the next four largest Laplacian spectral radii together with the corresponding graphs.

1. Introduction

Let $G=(V_G,E_G)$ be a simple graph with vertex set V_G and edge set E_G. $n=|G|$ $(=|V_G|)$ is the order of G. $A(G)$ denotes the $(0,1)$-adjacency matrix of G, while $D(G)=\mathrm{diag}(d_1,d_2,\ldots,d_n)$ denotes the matrix of vertex degrees (so $d_v=\deg(v)$). $L(G)=D(G)-A(G)$ is called the *Laplacian matrix* of G. It is well known that $L(G)$ is a symmetric and positive semi-definite matrix, and also singular (since its row sums are 0). Let $\mu_1(G)\geqslant\mu_2(G)\geqslant\cdots\geqslant\mu_n(G)=0$ be the eigenvalues of G given in non-increasing order. The largest eigenvalue of G $(=\mu_1(G))$ is called the *Laplacian spectral radius* of G, and is denoted by $\mu(G)$. Let $\mathbf{x}=(x_1,x_2,\ldots,x_n)^T$ be an eigenvector of G corresponding to $\mu(G)$. It will be convenient to associate a labelling of vertices of G (with respect to $\mathbf{x}$) in which x_v is a label of v. The *Laplacian characteristic polynomial* of G, equal to $\det(xI-L(G))$, is denoted by $\varphi(G,x)$ (or, for short, by $\varphi(G)$). For more details on graph spectra, see, for example, [1].

The Laplacian spectral radius of G is related to numerous (spectral or non-spectral) invariants of G, and has applications in various disciplines, like theoretical chemistry, combinatorial optimization, communication networks, etc. (see, for example, [2]). Since $\mu_1(G)+\mu_{n-1}(\overline{G})=n$, it is related to the *algebraic connectivity*, i.e. to the second smallest eigenvalue (here $\overline{G}$ stands for the complement of G); for more details, see [3] and references therein; in the case of bicyclic graphs, see [4]. Further on we will suppress graph names from our notation whenever they are understood from the context.

Recently, the problem concerning graph(s) with maximal (or minimal) Laplacian spectral radius within a given class of graphs has attracted much attention in the literature. Gutman [5] proved that the star has the largest Laplacian spectral radius in the class of n-vertex trees, while Petrović and Gutman [6] proved that the path has the smallest Laplacian spectral radius in the same class. Zhang and Li [7], and Guo [8] determined the first four n-vertex trees with largest Laplacian spectral radius, while Yu et al. [9] extended these results by determining the fifth to eighth trees with largest Laplacian

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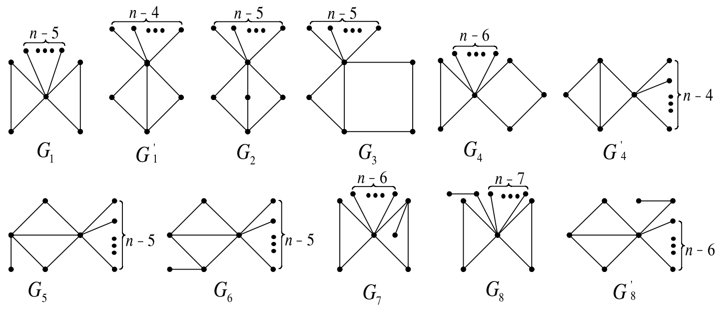

Fig. 1. Graphs $G_1, G_2, \dots, G_8, G_1', G_4'$ and G_8'.

spectral radius. Some further results on n-vertex trees with various invariants prescribed, like matching number (see [8,10]), pendant number (see [11]), and diameter (see [12]), are obtained in the literature. Guo [13] determined, in the class of n-vertex unicyclic graphs, the first four largest Laplacian spectral radii together with the corresponding graphs. Liu et al. [14] extended this ordering in the same class of graphs by determining the fifth to the ninth largest Laplacian spectral radii together with the corresponding graphs. Guo [15] determined the graphs with largest Laplacian spectral radius in the class of n-vertex unicyclic and bicyclic graphs having the fixed number of pendant vertices.

He et al. [16] determined the first four largest Laplacian spectral radii in the class of n-vertex bicyclic graphs together with the corresponding graphs (see the graphs $G_1, G_1', G_2, G_3, G_4, G_4'$ of Fig. 1). It turns that all these graphs have spectral radius greater than $n-1$. In this paper, we first identify all remaining graphs whose Laplacian spectral radius is in the closed interval $[n-1, n]$ (see the graphs G_5, G_6, G_7, G_8, G_8' of Fig. 1), and then extend the above ordering by determining the fifth to eighth largest Laplacian spectral radii together with the corresponding graphs.

The remainder of the paper is organized as follows. In Section 2, we introduce some results from the literature to make the paper more self-contained. In Section 3, we identify the n-vertex bicyclic graphs whose Laplacian spectral radius is in the closed interval $[n-1, n]$ (all graphs from Fig. 1). In Section 4, we order all latter graphs by ordering the additional graphs (last five graphs from Fig. 1). In Appendix, we add some code in *Mathematica* to put more light on some details appearing in the proof of Lemma 4.3 (from Section 4).

2. Preliminaries

Throughout the paper, $G - v$ and $G - uv$ denote the graph obtained from G by deleting a vertex $v \in V_G$, or an edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex, or edge, is deleted). Similarly, $G + v$ and $G + uv$ are obtained from G by adding a vertex $v \notin V_G$, or an edge $uv \notin E_G$, respectively (note, if a vertex v is added to G, then its neighbours in G should be specified somehow). Recall, a connected n-vertex graph is bicyclic if it has $n+1$ edges. $\mathscr{B}_n$ denotes the set of all n-vertex bicyclic graphs.

Further on we will need the following lemmas.

Lemma 2.1 (*[17]*). *Let G be a connected graph on $n \geq 2$ vertices, and maximum degree $\Delta(G)$. Then $\mu(G) \geqslant \Delta(G) + 1$, with equality if and only if $\Delta(G) = n - 1$.*

Let $N(v) = \{w \in V_G \mid vw \in E_G\}$. Clearly, $\deg(v) = |N(v)|$—recall that $d_i = \deg(v_i)$.

Lemma 2.2. *Let G be a bicyclic graph on n vertices, and let v_i and v_j be any two vertices of G. If v_i and v_j are adjacent then $d_i + d_j \leqslant n + 2$; otherwise, $d_i + d_j \leqslant n + 1$.*

Proof. Note first that G (as a bicyclic graph) has just two independent cycles. Therefore, we have:

If $v_iv_j \in E_G$, then $|N(v_i) \cup N(v_j)| \leq n$, $|N(v_i) \cap N(v_j)| \leq 2$. Hence,

$$d_i + d_j = |N(v_i) \cup N(v_j)| + |N(v_i) \cap N(v_j)| \leq n + 2.$$

If $v_iv_j \notin E_G$, then $|N(v_i) \cup N(v_j)| \leq n - 2$, $|N(u_i) \cap N(u_j)| \leqslant 3$. Hence,

$$d_i + d_j = |N(v_i) \cup N(v_j)| + |N(v_i) \cap N(v_j)| \leq n + 1.$$

This completes the proof. $\square$

Let $m_i = \frac{\sum_{v_iv_j \in E_G} d_j}{d_i}$ be the *average 2-degree* of a vertex v_i (of G).

Lemma 2.3 (*[18]*). *Let G be a graph on $n > 1$ vertices. Then*

$$\mu(G) \leqslant \max\{d_i + m_i \mid v_i \in V_G\}.$$

Lemma 2.4 *([19]). Let G be a graph on $n \geq 2$ vertices. Then*

$$\mu(G) \leq \max\{d_i + d_j - |N(v_i) \cap N(v_j)| \mid v_i v_j \in E_G\}. \tag{2.1}$$

Lemma 2.5 *([20]). Let G be a graph on n vertices. Then $\mu(G) \leq n$ with the equality if and only if $\overline{G}$ is disconnected, where $\overline{G}$ is the complement of G.*

Let $L_v(G)$ be the principal submatrix of $L(G)$ obtained from $L(G)$ by deleting the row and the column corresponding to the vertex v.

Lemma 2.6 *([16]). Let G be a connected rooted graph on n vertices and root r, which consists of a subgraph H (with at least two vertices) and $n - |H|$ pendant edges (neither in H) attached at vertex v of H (note, $|H|$ denotes the order of H). Then*

$$\varphi(G, x) = (x-1)^{n-|H|}\varphi(H, x) - (n - |H|)x(x-1)^{n-|H|-1}\varphi(L_v(H), x).$$

3. Bicyclic graphs with $\mu(G) \in [n-1, n]$

In this section, we will prove that the graphs from Fig. 1 are all bicyclic n-vertex graphs whose spectral radius is in the closed interval $[n-1, n]$. The following two lemmas are of crucial importance:

Lemma 3.1. *Let G be a graph on $n \geq 2$ vertices with $\mu(G) \in [n-1, n]$. Then G contains two adjacent vertices which cover all its vertices, except possibly one.*

Proof. If $d_v + d_u - |N(u) \cap N(v)| < n - 1$ for every edge $uv \in E_G$, then (by Lemma 2.4) $\mu(G) < n - 1$, a contradiction. Consider now an edge pq such that $d_p + (d_q - |N(p) \cap N(q)|) \geq n - 1$. Then it follows that p covers all its neighbours (with q included), and q covers all its neighbours not covered by p (now with p included).

This completes the proof. □

So it follows that G (with $\mu(G) \geq n-1$) consists of two adjacent vertices, say a and b, which cover all vertices of G except possibly one, say c. For the sake of simplicity, we assume that $\Delta(G) < n - 1$ (otherwise, $\mu(G) = n$, by Lemma 2.5). If G is a bicyclic graph, then we can say more:

Lemma 3.2. *Under the above assumptions on G, if $n \geq 11$ then d_a or d_b is greater than or equal to $n - 2$.*

Proof. By Lemma 2.3, there exists at least one vertex in G (say v) such that $d_v + m_v \geq n - 1$. If $d_v = 1$, let w be its (unique) neighbour. Then $d_w \geq n - 2$, and we are done if w is equal to a, or to b. Otherwise, by Lemma 3.1, the only uncovered case arises if $v = c$ and $w \in N(a) \cup N(b)$, but then (since G is bicyclic) $d_w \leq 4$, and so too small. Therefore, we next assume that $d_v > 1$.

Let $N(v) = \{w_1, w_2, \ldots, w_d\}$, where $d = d_v$. Then $d_v + m_v = d + \frac{1}{d}\sum_{i=1}^{d} d_{w_i}$. If $d = 2$ then $d_v + m_v \leq 2 + \frac{n+2}{2}$ (by Lemma 2.2). But then $d_v + m_v < n - 1$ for $n > 8$, and consequently $d_v \neq 2$. If $d = 3$ then $d_v + m_v \leq 3 + \frac{n+2+4}{3}$ (note that $d_{w_1} + d_{w_2} \leq n + 2$ by Lemma 2.2); on the other hand, since we can take that $w_3 \neq a, b$, then $d_{w_3} \leq 4$. But then $d_v + m_v < n - 1$ for $n > 9$, and consequently $d_v \neq 3$. Extending the above arguments, we get that $d_v \neq 4$ (for $n > 10$).

In what remains, $d_v > 4$, and so v is equal to a or b, say $v = a$. Now we can take that $d_a + m_a \leq d + \frac{n+3}{d}$ (note, $\sum_{i=1}^{d} d_{w_i} \leq (n+1) + 2$, since G has $n + 1$ edges, and at most two are counted twice). If the last quantity is less than $n - 1$ we are done. Otherwise, we have that $d + \frac{n+3}{d} \geq n - 1$ holds. Solving a corresponding quadratic equation in d we obtain

$$d \geq \frac{n - 1 + \sqrt{(n-1)^2 - 4(n+3)}}{2}. \tag{3.2}$$

For $n > 9$ we have that $d > n - 3$, and thus $d = n - 2$ (note $d < n - 1$). Notice also that the other region for d can be rejected since then $d < 3$.

This completes the proof. □

Without loss of generality, assume that $d_a \geq d_b$. Then, from Lemma 3.2, it follows that $d_a = n - 2$ or $n - 1$.

Collecting the above structural properties of G we easily get that G is one of the graphs from Fig. 1. Namely, G_1 and G_1' have maximum degree equal to $n - 1$. For all others, the maximum degree is $n - 2$. Observing vertex c we have: G_2 is a unique graph with $d_c = 3$; G_3, G_4 and G_4' are the graphs with $d_c = 2$; G_5, G_6, G_7, G_8 and G_8' are the graphs with $d_c = 1$. Note also that we assumed here that a and c are non-adjacent, while b and c can be taken to be, or not to be adjacent. (That means that the choice of a and b is not unique.) So we arrive at the following result:

Theorem 3.3. *If G is a bicyclic n-vertex graph (with $n \geq 11$) whose Laplacian spectral radius is in the closed interval $[n-1, n]$, then G is one of the graphs from Fig. 1.*

4. The ordering of graphs in $\{G_5, G_6, G_7, G_8, G_8'\}$

In this section, we order graphs G_5, G_6, G_7, G_8, G_8' (from Fig. 1) according to their Laplacian spectral radius. In what follows the following results are important:

Lemma 4.1. *If G is a bicyclic graph of order $n \geqslant 11$, then $\mu(G_8') = \mu(G_8)$ is the largest root of the equation $h_8(x) = 0$, where*

$$h_8(x) = x^3 - (n+2)x^2 + (3n-2)x - n$$

and $\mu(G_i)$ is the largest root of the equation $h_i(x) = 0$ $(i = 5, 6, 7)$, where

$$h_5(x) = x^4 - (n+6)x^3 + (7n+4)x^2 - (11n-6)x + 4n;$$
$$h_6(x) = x^5 - (n+8)x^4 + (9n+17)x^3 - 2(13n+1)x^2 + (27n-13)x - 8n;$$
$$h_7(x) = x^4 - (n+5)x^3 + 3(2n+1)x^2 - (9n-5)x + 3n.$$

Proof. By the routine calculations based on Lemma 2.6, we easily obtain:

$$\varphi(G_5, x) = x(x-1)^{n-6}(x-2)\left[x^4 - (n+6)x^3 + (7n+4)x^2 - (11n-6)x + 4n\right],$$
$$\varphi(G_6, x) = x(x-1)^{n-6}\left[x^5 - (n+8)x^4 + (9n+17)x^3 - 2(13n+1)x^2 + (27n-13)x - 8n\right],$$
$$\varphi(G_7, x) = x(x-1)^{n-6}(x-3)\left[x^4 - (n+5)x^3 + 3(2n+1)x^2 - (9n-5)x + 3n\right],$$
$$\varphi(G_8, x) = x(x-1)^{n-6}(x-2)(x-4)\left[x^3 - (n+2)x^2 + (3n-2)x - n\right],$$
$$\varphi(G_8', x) = x(x-1)^{n-6}(x-3)^2\left[x^3 - (n+2)x^2 + (3n-2)x - n\right].$$

The rest of the proof easily follows. □

Lemma 4.2. *Let G_5, G_6, G_7 and G_8 be the graphs (on n vertices) from Fig. 1. Then*

$$\mu(G_5) > \mu(G_6), \qquad \mu(G_6) > \mu(G_8) \quad \text{and} \quad \mu(G_7) > \mu(G_8).$$

Proof. Note first that $\mu(G_i) \in (n-1, n)$ for $i = 5, 6, 7, 8$ (namely, by Lemma 2.1, $\mu(G_i) \neq n-1, n$). From the previous lemma we obtain

$$\varphi(G_5, x) - \varphi(G_6, x) = x(x-1)^{n-6}[x(x-1)(n-1-x)] < 0$$

for $x \in (n-1, n)$. Therefore $\mu(G_5) > \mu(G_6)$.

Similarly, we have

$$\varphi(G_6, x) - \varphi(G_8, x) = x^2(x-1)^{n-6}(x-3)(n-1-x) < 0$$

for $x \in (n-1, n)$. Therefore $\mu(G_6) > \mu(G_8)$.

Finally, we have

$$\varphi(G_7, x) - \varphi(G_8', x) = x(x-1)^{n-6}(x-n) < 0$$

for $x \in (n-1, n)$. Therefore $\mu(G_7) > \mu(G_8') = \mu(G_8)$.

This completes the proof. □

The proof of the next lemma is more involved.

Lemma 4.3. *Let G_6 and G_7 be the graphs (on n vertices) from Fig. 1. Then*

$$\mu(G_6) > \mu(G_7).$$

Proof. Recall first that $\mu(G_i)$ is the largest root of $h_i(x)$ $(i = 6, 7)$. We first note that $h_i(x)$ cannot have two roots greater than $n-1$. Otherwise, the coefficient of the second largest term will be greater than $2n-2$ in modulus, and this is not the case if $n \geqslant 11$; recall that all roots of $h_i(x)$ are positive (cf. Lemma 4.1).

We first claim that $\lim_{n\to+\infty}[\mu(G_i) - (n-1)] = 0$ for $i = 6, 7$.[1]

Let $T_i(x-(n-1))$ be the Taylor's polynomial for $h_i(x)$ at point $n-1$. Putting $y = x-(n-1)$, we get

$$T_6(y) = -15 + 8n - n^2 + \left(79 - 112n + 59n^2 - 13n^3 + n^4\right)y + \left(-111 + 118n - 39n^2 + 4n^3\right)y^2 + \left(59 - 39n + 6n^2\right)y^3 + (-13+4n)y^4 + y^5,$$

[1] The same holds for $i = 5$, i.e. for G_5 in the role of G_6, or G_7—the proof is analogous.

and

$$T_7(y) = 4 - n + \left(-20 + 24n - 9n^2 + n^3\right) y + \left(24 - 18n + 3n^2\right) y^2 + (-9 + 3n)y^3 + y^4.$$

In this way, instead of intervals $(n-1, n)$ for the largest roots of $h_i(x)$, we will consider interval $(0, 1)$ and zeros of $T_i(y)$in this interval.

Define now two sequences (a_n) and (b_n) as follows:

$$a_n = \frac{15 - 8n + n^2}{79 - 112n + 59n^2 - 13n^3 + n^4}, \qquad b_n = \frac{-4 + n}{-20 + 24n - 9n^2 + n^3}.$$

Note that at these points the linear terms of $T_6(y)$ and $T_7(y)$ are vanishing, respectively. On the other hand, we have that $T_6(a_n) > 0$ and $T_7(b_n) > 0$ (whenever $n \geqslant 11$). So $0 < \mu(G_6) - (n-1) < a_n$ and $0 < \mu(G_7) - (n-1) < b_n$. Since (a_n) and (b_n) are 0-sequences, we are done (i.e. the claim holds).

We will now describe our ad hoc strategy to prove that $\mu(G_7) < \mu(G_6)$.

For this aim we will construct yet another sequence, say (c_n), which separates $\mu(G_7)$ and $\mu(G_6)$. More precisely, we choose (c_n) such that $\mu(G_7) < c_n < \mu(G_6)$ for each $n \geqslant 11$. To prove this it suffices to prove that $T_6(c_n) < 0$ (which implies that $c_n < \mu(G_6)$), and $T_7(c_n) > 0$ (which implies that $\mu(G_7) < c_n$).

One way to find (c_n) is as follows: consider $z = T_7(y)$ as a curve (in (y, z)-plane), then construct a tangent at point $y = b_n$, and take c_n to be its intersection with y-axes.

For this aim, we will use some Computer Algebra System (say *Mathematica*) to perform routine, but tedious calculations. Using this facilities we have obtained that

$$c_n = \frac{p_n}{q_n},$$

where

$$\begin{aligned} p_n = {} & -508672 + 2723200n - 6593088n^2 + 9540824n^3 - 9205133n^4 + 6256674n^5 \\ & - 3084816n^6 + 1118004n^7 - 298053n^8 + 57761n^9 - 7913n^{10} + 726n^{11} - 40n^{12} + n^{13} \end{aligned}$$

and

$$\begin{aligned} q_n = {} & -1831680 + 12683136n - 39342960n^2 + 72945920n^3 - 90804120n^4 + 80658564n^5 - 52954663n^6 \\ & + 26219871n^7 - 9887517n^8 + 2843263n^9 - 618987n^{10} + 100263n^{11} - 11704n^{12} + 930n^{13} - 45n^{14} + n^{15}. \end{aligned}$$

The corresponding code in *Mathematica* is given in Appendix (see I).

Now we have to compute the values of $T_6(y)$ and $T_7(y)$ at point c_n. Using again *Mathematica*, we have obtained that

$$T_6(c_n) = \frac{894062687731616418715140934860\,8 + \cdots - n^{73}}{-2061807034574650379788615680000\,0 + \cdots + n^{75}} < 0$$

and

$$T_7(c_n) = \frac{1237687063658927484829696 + \cdots + 27n^{52}}{1125637138896887218176000\,0 + \cdots + n^{60}} > 0.$$

The above expressions are given in the condensed form in order to give an indication that our latest claims on the signs hold at least asymptotically. Clearly, the exact values are not given due to space limitations.

The corresponding code in *Mathematica* is given in Appendix (see II).

This completes the proof. $\square$

Appendix

In this section, we give the code in *Mathematica* which is mentioned in the proof of Lemma 4.3.

```
(* Mathematica code *)

(* Commands to define h-polynomials and obtain their Taylor's polynomials at
   point n-1 *)

h6[x_,n_] := x^5 - (n+8)*x^4 + (9n+17)*x^3 - 2(13n+1)*x^2 + (27n-13)*x - 8n
h7[x_,n_] := x^4 - (n+5)*x^3 + 3(2n+1)*x^2 - (9n-5)*x + 3n

T6 = Series[h6[(n-1)+y, n], {y, 0, 5}] //Normal
```

```
T7 = Series[h7[(n-1)+y, n], {y, 0, 4}] //Normal

(* Commands to obtain a-sequence and b-sequence *)

a = -Coefficient[T6, y, 0] / Coefficient[T6, y, 1] //Simplify
b = -Coefficient[T7, y, 0] / Coefficient[T7, y, 1] //Simplify
```

(I): *Calculations related to sequence* (c_n).

```
(* Command to obtain c-sequence *)

c = X /. Solve[(Series[T7, {X, b, 1}] //Normal) == 0, X] //First //Together;

(* Commands to obtain values of polynomials T6 and T7 at point y = c
   [they are rational functions in n];
   next four commands give their numerators and denominators *)

T6c = T6 /. y -> c //Together;
T7c = T7 /. y -> c //Together;

T6cNum = Numerator[T6c]
T7cNum = Numerator[T7c]
T6cDen = Denominator[T6c]
T7cDen = Denominator[T7c]
```

(II): *Calculations to verify that* $T_6(c_n) < 0$ *and* $T_7(c_n) > 0$.

```
(* Commands to verify that T6c < 0 and T7c > 0, for n > 10  *)

Simplify[T6c < 0, n > 10]  (* the answer is yes *)
Simplify[T7c > 0, n > 10]  (* the answer is yes *)

(* An alternative proof that T6c < 0 and T7c > 0 for n > 6
[by using poles and zeros of T6c and T7c] *)

Max[Select[n /. Solve[T6cNum == 0, n], (# \[Element] Reals) &]] //N

Max[Select[n /. Solve[T6cDen == 0, n], (# \[Element] Reals) &]] //N

Max[Select[n /. Solve[T7cNum == 0, n], (# \[Element] Reals) &]] //N

Max[Select[n /. Solve[T7cDen == 0, n], (# \[Element] Reals) &]] //N

(* In all these cases it turns that the real roots of each numerator and
   each denominator are less than $6$, so that the leading coefficients were
   sufficient to determine the signs of corresponding polynomials in n,
   as is already confirmed for the asymptotic case *)
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